3. Calpuff Testing and Evaluation

Given the lack of formal guidance for implementation of the Calmet/Calpuff modeling system, Calpuff was tested to determine reasonable settings for control file options and parameters. A limited model performance evaluation was conducted to determine the utility of selected settings.

3.1 Calpuff Testing

John Vimont (NPS) provided initial advice on control file settings[11]. Default values were used when other information was not available (i.e., most of the time). Testing was conducted primarily to determine sensitivity of results and execution time associated with parameters/options for which default values were not provided. The goal was to achieve a technically competent implementation of the model while maintaining reasonable execution time.

Calpuff was tested using Calmet meteorological data files prepared as described in Section 2. Calpost was applied to summarize Calpuff hourly output. Values for selected Calpuff control file parameters/options were individually and systematically varied to determine effect on results and execution time.

Testing was conducted, for example, to determine sensitivity of results to deployment of puff splitting, terrain effects, PDF for convective conditions, and partial plume penetration of elevated inversion. All seemed to have some effect on model results but, with the exception of puff splitting, none of these options exacted a significant execution time penalty. Therefore, it was concluded appropriate to deploy all for production runs for major sources. Given the number of minor sources along with execution time considerations, puff splitting was not deployed for minor sources.

3.2 Calpuff Evaluation

To determine the effectiveness of selected Calpuff control file settings, as well as the utility of the NDDH Calmet/Calpuff implementation in general, a limited model performance evaluation was conducted. Model predictions were compared with observed concentrations for two SO_2 monitoring sites located in and near the Theodore Roosevelt National Park North Unit located in western North Dakota. The evaluation was limited in that full AMS statistics were not generated, and predictions/observations were not paired in time.

The NDDH Calpuff evaluation is described in the report in Appendix B. Predicted-to-observed comparisons were made on the basis of the highest value, second-high value, and average of top ten values for each year of meteorological data (1990-1994) for 1-hour, 3-hour, and 24-hour averaging periods. Using control file settings established in the testing process, the model performed well, with virtually all of the predicted/observed comparisons falling within a factor of two, and no significant overprediction/underprediction bias.

The testing and evaluation process resulted in final control file settings for Calpuff, as summarized in Table 3-1.

Table 3-1
Calpuff Control File

Parameter/Option	Value
No. chemical species	5
Vertical distribution near field	1
Terrain adjustment method	3
Subgrid-scale complex terrain	0
Slug model	No
Transitional plume rise	Yes
Stack tip downwash	Yes
Vertical wind shear	No
Puff splitting	Yes
Chemical mechanism	1
Wet removal	Yes
Dry deposition	Yes
Dispersion coefficient method	2
Partial plume penetration - elev. inversion	Yes
PDF used under convective conditions	Yes
CSPEC	SO_2, SO_4, NO_x, HNO_3, NO_3
Chemical parameters - dry gas deposition	Default
Size parameters - dry particle deposition	Default
RCUTR	30.
RGR	10.
REACTR	8.
NINT	9
IVEG	2
Wet deposition parameters	Default
Ozone data input option	1
Background ammonia conc. (ppb)	1.

Table 3-1 (Cont.)
Calpuff Control File

Parameter/Option	Value
SYTDEP	550.
MHFTSZ	0
JSUP	5
XSAMLEN	0.25
MXNEW	99
MXSAM	99
Maximum mixing height (m)	4000.
Minimum mixing height (m)	20.
NSPLIT	3
IRESPLIT	Hour 17-22 = 1
ZISPLIT (m)	100.
ROLOMAX	0.25

4. Calpuff Modeling - PSD Class I Increments

The Calmet/Calpuff modeling system, as implemented by NDDH, was used to evaluate impact of proposed ambient emission increases at the MRY station on PSD Class I increments. Based on preliminary modeling, it was determined that NO_x and PM_{10} emission increases at MRY would not significantly impact PSD increments at Class I areas, using Class I significance levels implemented by the NDDH[3]. Therefore, the Calpuff modeling analysis for the MRY station was limited to an assessment of SO_2 increments.

All North Dakota Class I areas, including Lostwood Wilderness Area and all three units of the Theodore Roosevelt National Park, were modeled. The Medicine Lake and Fort Peck Class I areas in Montana were also modeled, but with limited receptor resolution.

The MRY station Class I increment modeling analysis utilized all five years of Calmet processed meteorological data (1990-1994).

4.1 Source Data

Based on NDDH policy, the emission inventory for the Class I increment analysis included all major PSD sources located within 250 km of each Class I area, and all minor PSD sources located within 50 km of each Class I area. Major SO_2 sources (North Dakota and Montana) include primarily electrical generating stations and natural gas processing plants. Minor sources (North Dakota) are primarily oil and gas production facilities. Because of the relatively small number of major sources, a generic major-source inventory (i.e., all sources located within 250 km of at least one subject Class I area) was prepared and used for modeling all Class I areas. Because of the large number of minor sources (over 2000 wells statewide), a unique minor-source inventory was prepared for each Class I area (i.e., all sources located within 50 km of subject Class I area). Using the NDDH postprocessing system, described in Section 4.4, Calpuff results for minor sources were added to those for major sources.

Even though numerous oil and gas production facilities are found in the vicinity of Medicine Lake and Fort Peck Class I areas, emission/stack data were not obtainable for such facilities located in Montana. Therefore, the local minor-source contribution was not accounted for in Calpuff modeling for Montana Class I areas, and model predictions for these areas may accordingly be understated.

Major and minor source locations are depicted in Figure 4-1. The major-source inventory is provided in Table 4-1. Information on minor sources can be obtained from Calpuff input files provided on

Figure 4-1: Source Locations and Class I Areas

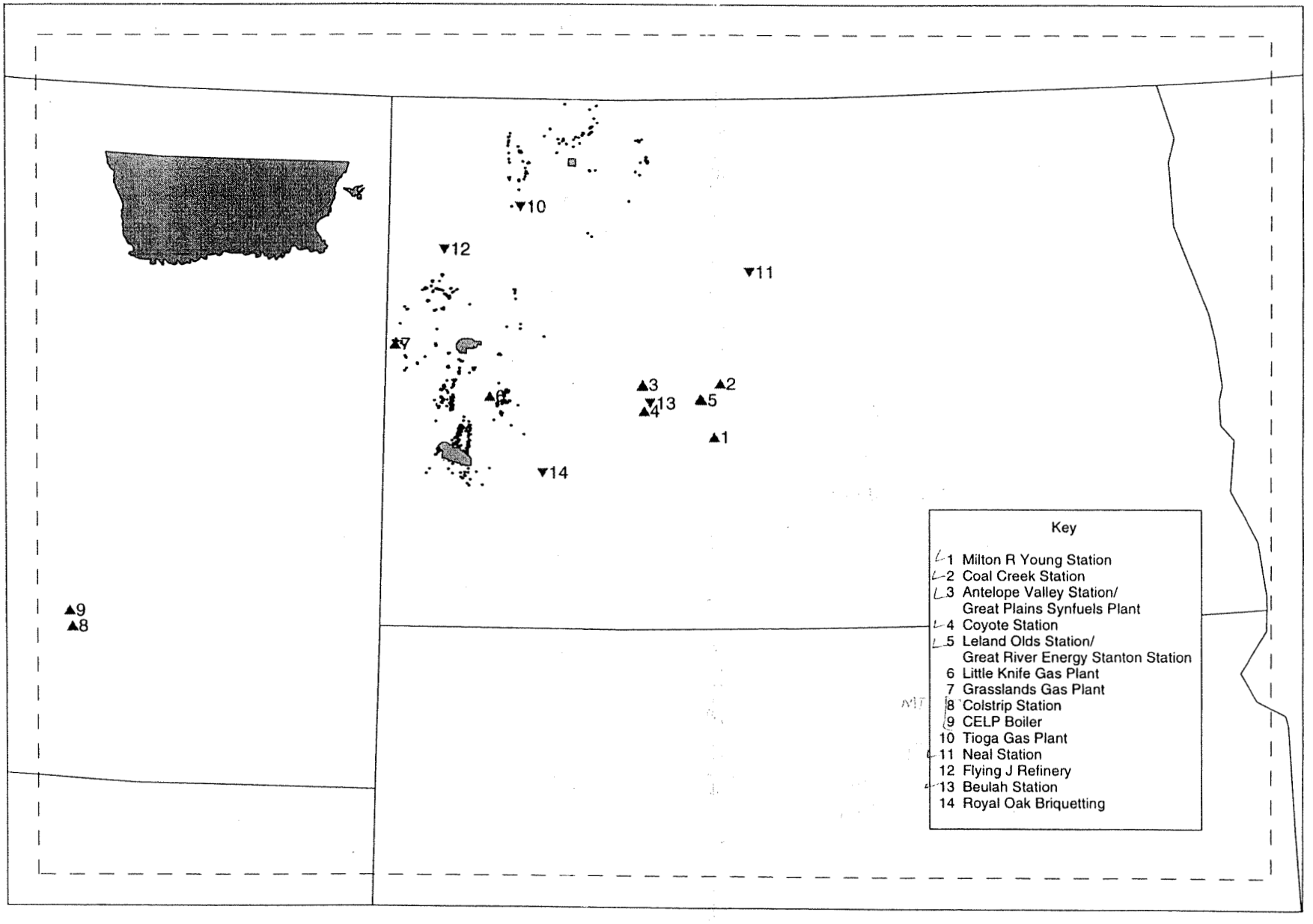


Table 4-1
Major Source Inventory for Class I Increment Analysis

Source No.	X Coordinate (km)	Y Coordinate (km)	Stack Height (m)	Base Elevation (m)	Stack Diameter (m)	Exit Vel. (m/s)	Exit Temp. (deg. K)	Bldg. Dwash	Emission Rate (SO2)	
1	! SRCNAM = Milton R Young Station Unit 1 (3hr, 24hr) !									
1	! X =	59.519,	341.409,	91.4,	597.4,	5.8,	21.3,	455.0,	0.,	264.6 ! !END!
2	! SRCNAM = Milton R Young Station Unit 2 (3hr, 24hr) !									
2	! X =	59.462,	341.356,	167.6,	597.4,	7.6,	20.3,	347.0,	0.,	242.6 ! !END!
3	! SRCNAM = Milton R Young Station Unit 1 (Annual) !									
3	! X =	59.519,	341.409,	91.4,	597.4,	5.8,	21.3,	455.0,	0.,	832.5 ! !END!
4	! SRCNAM = Milton R Young Station Unit 2 (Annual) !									
4	! X =	59.462,	341.356,	167.6,	597.4,	7.6,	20.3,	347.0,	0.,	242.6 ! !END!
5	! SRCNAM = Coal Creek Station Units 1+2 !									
5	! X =	63.487,	375.784,	201.,	602.,	6.7,	27.2,	383.,	0.,	1596.6 ! !END!
6	! SRCNAM = Antelope Valley Station Units 1+2 !									
6	! X =	12.459,	374.908,	182.9,	588.3,	7.0,	22.3,	356.3,	0.,	484.4 ! !END!
7	! SRCNAM = Great Plains Synfuels Plant Main !									
7	! X =	12.095,	373.994,	121.9,	588.3,	7.01,	14.2,	361.8,	0.,	407.0 ! !END!
8	! SRCNAM = Great Plains Synfuels Plant T.O. !									
8	! X =	12.095,	373.994,	61.0,	588.3,	4.42,	1.5,	972.8,	0.,	11.5 ! !END!
9	! SRCNAM = Coyote Station !									
9	! X =	13.513,	357.842,	152.0,	556.9,	6.4,	29.3,	369.7,	0.,	672.2 ! !END!
10	! SRCNAM = Leland Olds Station Unit 1 (3hr, 24hr) !									
10	! X =	51.326,	365.208,	106.7,	518.3,	5.3,	16.7,	452.0,	0.,	271.7 ! !END!
11	! SRCNAM = Leland Olds Station Unit 2 (3hr, 24hr) !									
11	! X =	51.326,	365.208,	152.4,	518.3,	6.7,	20.9,	450.0,	0.,	466.2 ! !END!
12	! SRCNAM = Leland Olds Station Unit 1 (Annual) !									
12	! X =	51.326,	365.208,	106.7,	518.3,	5.3,	16.7,	452.0,	0.,	78.1 ! !END!
13	! SRCNAM = Leland Olds Station Unit 2 (Annual) !									
13	! X =	51.326,	365.208,	152.4,	518.3,	6.7,	20.9,	450.0,	0.,	306.3 ! !END!
14	! SRCNAM = Great River Energy Stanton Station (3hr) !									
14	! X =	50.407,	365.773,	77.7,	518.3,	4.6,	27.2,	404.,	0.,	172.5 ! !END!
15	! SRCNAM = Little Knife Gas Plant !									
15	! X =	-82.767,	367.223,	59.5,	780.5,	1.8,	10.0,	755.0,	0.,	53.8 ! !END!
16	! SRCNAM = Grasslands Gas Plant (3hr) !									
16	! X =	-149.696,	401.234,	65.0,	615.9,	0.86,	20.6,	581.1,	0.,	64.5 ! !END!
17	! SRCNAM = Grasslands Gas Plant (24hr, Annual) !									
17	! X =	-149.696,	401.234,	65.0,	615.9,	0.86,	20.6,	581.1,	0.,	34.4 ! !END!
18	! SRCNAM = Colstrip Station (3hr) !									
18	! X =	-357.648,	220.211,	210.9,	988.7,	7.3,	33.8,	363.2,	0.,	538.0 ! !END!
19	! SRCNAM = Colstrip Station (24hr, Annual) !									
19	! X =	-357.648,	220.211,	210.9,	988.7,	7.3,	33.8,	363.2,	0.,	344.0 ! !END!
20	! SRCNAM = CELP Boiler !									
20	! X =	-359.424,	230.411,	61.0,	945.1,	2.5,	22.6,	433.2,	0.,	52.9 ! !END!
21	! SRCNAM = Tioga Gas Plant (inc. expanding) !									
21	! X =	-67.762,	489.627,	30.5,	686.0,	1.7,	7.7,	782.0,	0.,	62.9 ! !END!
22	! SRCNAM = Neal Station Units 1+2 (inc. expanding !									
22	! X =	82.646,	447.977,	42.4,	488.0,	1.8,	25.0,	470.0,	0.,	37.4 ! !END!
23	! SRCNAM = Flying J Refinery Heaters+Boiler 2 (inc. expanding) !									
23	! X =	-117.411,	462.238,	17.3,	575.0,	0.9,	3.2,	700.0,	0.,	2.62 ! !END!
24	! SRCNAM = Flying J Refinery Boiler 1 (inc. expanding) !									
24	! X =	-117.411,	462.238,	30.2,	575.0,	1.2,	3.4,	464.0,	0.,	1.22 ! !END!
25	! SRCNAM = Flying J Refinery Boiler 3 (inc. expanding) !									
25	! X =	-117.411,	462.238,	9.1,	575.0,	0.8,	6.3,	464.0,	0.,	1.74 ! !END!
26	! SRCNAM = Beulah Station Boilers 1-2 (inc. expanding) !									
26	! X =	17.404,	362.995,	23.0,	567.0,	1.7,	7.6,	477.0,	0.,	28.0 ! !END!
27	! SRCNAM = Beulah Station Boilers 3-5 (inc. expanding) !									
27	! X =	17.404,	362.995,	30.5,	567.0,	2.1,	14.6,	527.0,	0.,	50.2 ! !END!
28	! SRCNAM = Royal Oak Briquetting Boilers 1-3 (inc. expanding) !									
28	! X =	-53.232,	318.050,	19.2,	751.0,	1.4,	9.8,	520.0,	0.,	12.7 ! !END!
29	! SRCNAM = Royal Oak Briquetting ACC (inc. expanding) !									
29	! X =	-53.232,	318.050,	26.2,	751.0,	3.35,	9.35,	1172.0,	0.,	56.2 ! !END!

computer media with this report. Emission/stack data for major sources was determined by NDDH permit engineers, while data for minor sources was obtained from the State Industrial Commission's Oil and Gas data base. Increment-expanding sources (sources which existed prior to baseline date and are now shut down) were included in the analysis and are designated in Table 4-1 (Sources 21-29). Emission rates for some major sources varied on the basis of averaging period, as also indicated in the table (if no averaging period is given, the entry applies to all averaging periods). For this reason (and others), major source facilities were modeled individually, and the results for Calpuff runs reflecting equivalent emission rate averaging periods were added using the NDDH postprocessing system described in Section 4.4. The postprocessing system also accommodated treatment of increment-expanding sources, whose contributions were subtracted from the total.

4.2 Receptor Locations

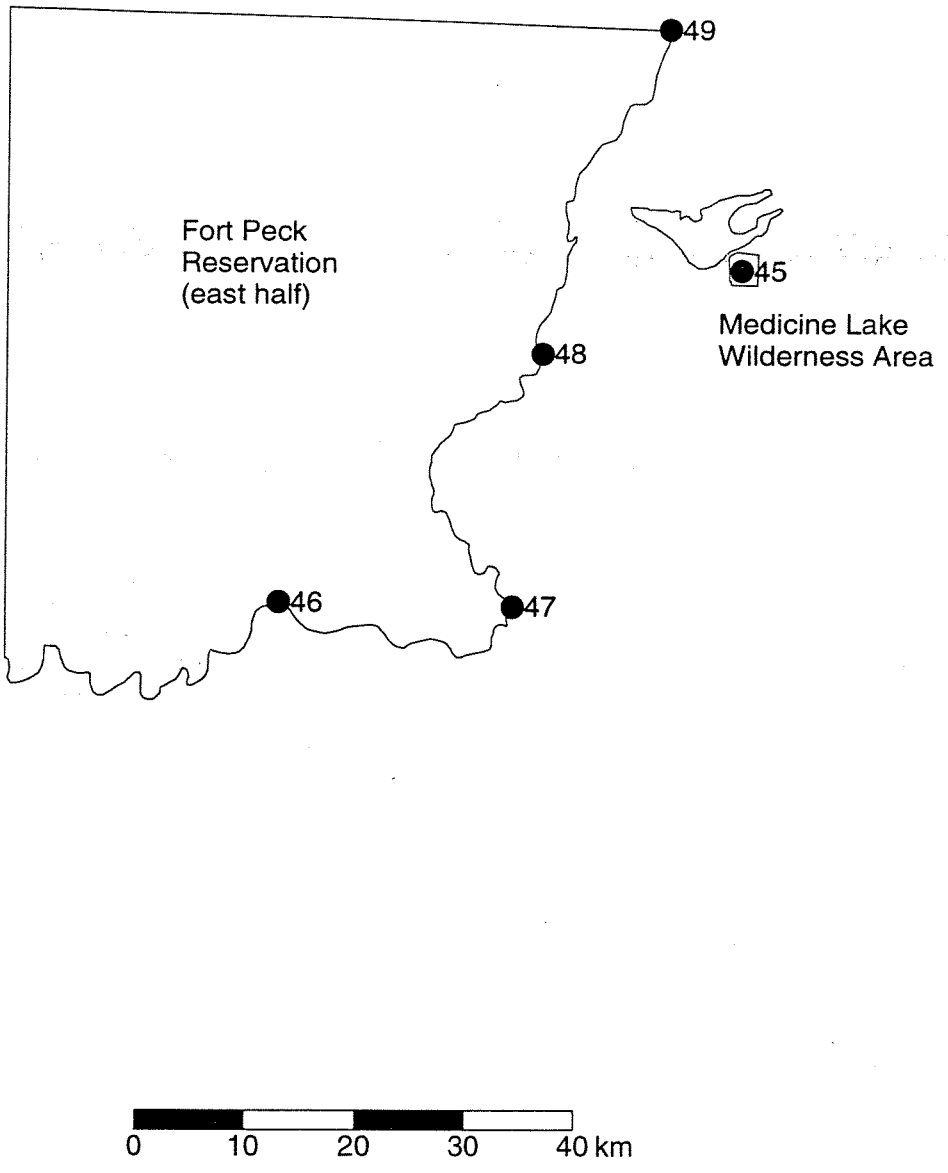
Receptor locations for the MRY station Class I Calpuff analysis are shown in Figures 4-2 and 4-3. Figure 4-2 identifies receptor locations for North Dakota Class I areas and Figure 4-3 depicts receptor locations for Montana Class I areas. Numbers in the figures correspond to the receptor numbering system employed in Calpuff input/output files. Receptor coverage includes 22 receptors (No. 1-22) at TRNP South Unit, 16 receptors (No. 23-38) at TRNP North Unit, 1 receptor (No. 39) at TRNP Elkhorn Ranch Unit, 5 receptors (No. 40-44) at Lostwood Wilderness Area, 1 receptor (No. 45) at Medicine Lake Wilderness Area, and 4 receptors (No. 46-49) at Fort Peck Reservation.

Maximum receptor spacing in North Dakota Class I areas is on the order of 4-5 kilometers. Given the distance of the largest-contributing sources from Class I areas (150-200 km), concentration gradients in the vicinity of Class I areas were not expected to be significant. Based on subsequent model execution which confirmed this expectation, receptor coverage was deemed sufficient.

Receptor coverage for Medicine Lake and Fort Peck Class I areas was limited because they are located even farther from largest-contributing sources, and (as indicated in Section 4.1) the local minor-source contribution could not be accounted for. Most of Fort Peck is located more than 300 km from major North Dakota sources. Also, some compromise in receptor resolution was necessary to achieve practical Calpuff execution times, and to accommodate the NDDH postprocessing system (Section 4.3).

4.3 Calpuff Execution and Postprocessing

Figure 4-3: Receptor Locations - Montana Class I Areas



Calpuff was executed with source and receptor data as outlined above, and with meteorological data developed as described in Section 2. Calpuff control file options/parameters were set based on recommendations from John Vimont[11], and on the NDDH testing/evaluation process described in Section 3. Default values were used to the extent possible. More significant control file settings for Calpuff are summarized in Table 3-1. The complete NDDH Calpuff input control file was provided on computer media with this report.

As shown in Table 3-1, the NDDH elected to use dispersion coefficients calculated from micrometeorological variables (MDISP Option 2) rather than default PG dispersion coefficients (MDISP Option 3). Use of MDISP Option 2 was thought to be more consistent with the dispersion treatment in AERMOD[12], and in other state-of-the-art models. In any event, the suitability of dispersion coefficients based on micrometeorological variables was confirmed in the testing/evaluation process described in Section 3.

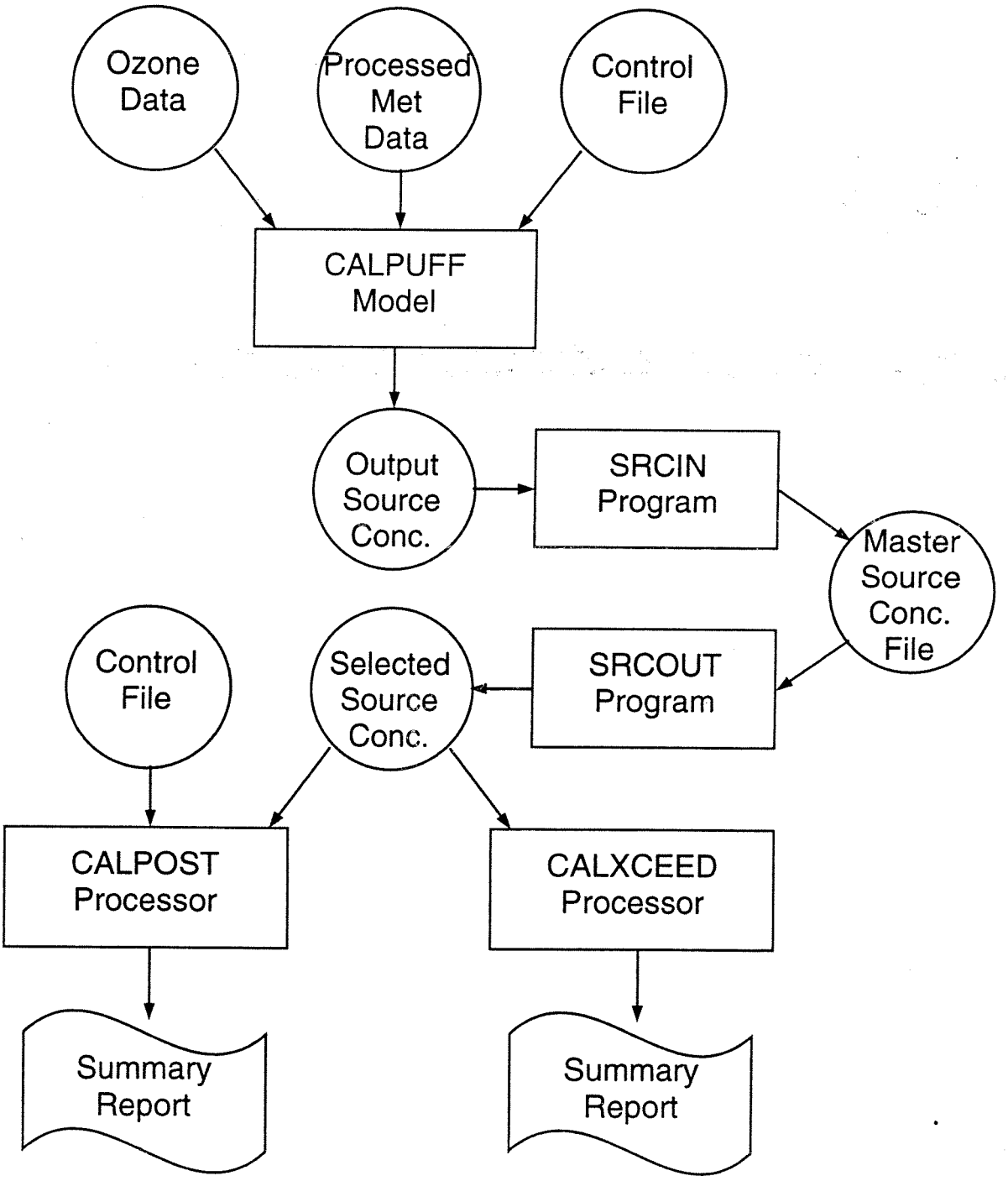
The NDDH also elected to deploy puff splitting for modeling major sources. Calpuff testing (Section 3.1) indicated that the puff splitting option can substantially increase model execution time. Therefore, puff splitting was not deployed for modeling the more numerous minor sources. Given source-receptor distances for minor sources compared with major sources (i.e., <50 km versus 100-200 km), and the fact that plumes associated with low-level minor-source emissions should tend to remain near the surface, puff splitting was thought to be less of an issue for minor sources anyway.

Calpuff execution included the option to provide hourly ozone data. Ozone data were obtained from a single, NDDH monitoring site located about 140 km east of TRNP Elkhorn Ranch Unit. Ozone data were concurrent with Calmet meteorological data (i.e., 1990-1994).

Calpuff processing as implemented by the NDDH is depicted in Figure 4-4. Major sources were modeled individually, while minor sources were modeled as a separate group for each Class I area. Calpuff hourly output for major sources, and minor source groups, was added to the Master Source Concentration File (SCF) via NDDH program SRCIN. Each major source, and minor source group, is stored as a separate layer in the SCF, which is a Fortran direct access file. SRCIN also converts hourly concentrations from increment-expanding sources to negative values before adding to the SCF. NDDH program SRCOUT sums hourly concentrations for selected source layers in the SCF, and converts the results to the original Calpuff output file format required by Calpost and Calxceed. Calpost was then applied in the conventional manner.

Figure 4-4

NDDH Calpuff Modeling System



Because Calpuff/Calpost was predicting numerous exceedances of Class I increments, it was necessary to determine if the MRY station contributes significantly to any of these predicted exceedances. While Calpost can provide the number of predicted exceedances of a threshold value at a given receptor, it does not provide the value of each exceedance, nor any information on source contributions. Therefore, the NDDH developed the Calxceed program. Calxceed lists the value of each exceedance, the contribution of an individual source (or source group) to each exceedance, the total number of exceedances, and the number of exceedances with significant individual source contributions. These parameters are provided for each receptor for each threshold level (currently hard-coded as 3-hour and 24-hour SO_2 Class I increments). Calxceed requires two Calpuff-compatible hourly concentration files: one representing cumulative concentrations and the other reflecting individual source (source group) concentrations. Calxceed was executed to complete the MRY station Class I increment analysis.

The complete NDDH Calpuff postprocessing system includes components for visualizing output (using gridded receptors), which were utilized in the MRY station analysis.

4.4 Results

Results of the Calpuff SO_2 modeling analysis for MRY station Class I increment consumption are summarized in Tables 4-2 and 4-3. Table 4-2 provides essential regulatory comparisons while Table 4-3 provides supplemental information on source contributions.

Table 4-2 provides the overall highest and highest, second-highest predictions for the five-year period of meteorological data. Values are provided for the worst-case year for each Class I area. Also provided in Table 4-2 is the maximum number of predicted exceedances of the applicable Class I increment (3-hour and 24-hour average) and the number of cases where MRY station significantly contributed to a predicted increment violation. Again, these values are provided for the worst-case receptor and year for each Class I area. Significant contributions are based on significant impact levels established by the NDDH[3]. Class I significant impact levels for SO_2 are 1.0 $\mu g/m^3$, 0.2 $\mu g/m^3$, and 0.1 $\mu g/m^3$ for 3-hour, 24-hour, and annual averages, respectively.

Table 4-2 summarizes Calpuff results for the five-year period modeled. Expanded results for individual years are provided in Appendix C.

The contributions of the MRY station and oil and gas facility (minor) sources to highest, second-highest predictions (3-hour and

Table 4-2
**Calpuff Class I Increment Results SO_2*
($\mu g/m^3$)**

	TRNP South	TRNP North	TRNP Elkhorn R.	Lostwood Wilderness	Med. Lake Wilderness	Ft. Peck Reservation
3-hr Predictions						
Highest	68.4	77.7	40.4	38.5	39.4	34.3
High, 2nd High	45.0	43.0	36.5	34.3	30.2	33.5
Max # of Exceedances**	7	9	2	5	2	2
Max # sig. MRY contrib. to violations**	4	8	0	4	1	1
24-hr Predictions						
Highest	15.0	18.3	13.6	9.1	10.6	10.5
High, 2nd High	13.4	12.7	13.2	8.6	7.1	7.4
Max # of Exceedances**	10	22	10	15	4	4
Max # sig. MRY contrib. to violations**	8	12	6	14	3	3
Max Annual Prediction	1.19	1.53	0.98	0.74	0.26	0.28

* PSD Class I increments for SO_2 are 25 $\mu g/m^3$, 5 $\mu g/m^3$, and 2 $\mu g/m^3$ for 3-hour, 24-hour, and annual averages, respectively.

** Worst-case receptor, year

Table 4-3
Calpuff Class I Increment Source Contributions
(μg/m³)

	TRNP South	TRNP North	TRNP Elkhorn R.	Lostwood Wilderness	Med. Lake Wilderness	Ft. Peck Reservation
3-hr Predictions						
High, 2nd High	45.0	43.0	36.5	34.3	30.2	33.5
MRY Contribution	1.5	2.9	0.5	5.2	5.2	2.6
Oil & Gas Contrib.	0.1	0.04	3.2	0.01	---	---
Overall Max Contrib.						
MRY Station	5.6	10.1	1.4	7.2	5.2	5.5
Oil & Gas Sources	14.1	17.7	3.2	0.2	---	---
24-hr Predictions						
High, 2nd High	13.4	12.7	13.2	8.6	7.1	7.4
MRY Contribution	1.1	0.8	0.7	1.5	1.0	1.0
Oil & Gas Contrib.	0.1	1.3	1.9	0.4	---	---
Overall Max Contrib.						
MRY Station	2.3	1.6	1.4	1.6	1.5	1.6
Oil & Gas Sources	7.0	9.6	2.9	0.5	---	---

24-hour) are summarized in Table 4-3. The highest, second-highest predictions reflect the worst-case year for each Class I area. Also shown in Table 4-3 is the overall highest contribution by MRY station, and by oil and gas sources, to predicted exceedances of the applicable Class I increment. These values reflect the highest contribution for the five modeled years at each Class I area.

As shown in Table 4-2, Calpuff predicts numerous exceedances of PSD Class I increments. The highest, second-highest 3-hour average prediction at Theodore Roosevelt National park (TRNP) is 45.0 $\mu g/m^3$ at the South Unit, which compares with the Class I increment of 25 $\mu g/m^3$. The highest, second-highest 24-hour average prediction (TRNP South Unit), 13.4 $\mu g/m^3$, compares with the Class I increment of 5 $\mu g/m^3$. The maximum number of increment exceedances (worst-case year and receptor) were found at TRNP North Unit, with 9 exceedances of the 3-hour increment and 22 exceedances of the 24-hour increment predicted. According to Calpuff results, the MRY station significantly contributed to (at most) eight 3-hour increment violations at TRNP North Unit, and fourteen 24-hour increment violations at Lostwood Wilderness Area.

The contributions of MRY station and oil and gas sources to the highest, second-highest prediction (3-hour and 24-hour average) at each Class I area is shown in Table 4-3. While these contributions are relatively small, particularly for oil and gas sources, the overall maximum contributions are much greater. As shown in Table 4-3, the maximum 3-hour contribution from MRY station is 10.1 $\mu g/m^3$ at TRNP North Unit. The maximum 24-hour contribution from MRY station is 2.3 $\mu g/m^3$ at TRNP South Unit. For oil and gas sources, the maximum contributions were 17.7 $\mu g/m^3$ and 9.6 $\mu g/m^3$ for 3-hour and 24-hour averages, respectively. For the ensemble of predicted increment exceedances, however,, the MRY station was generally a larger contributor, and more often a significant contributor, than oil and gas sources.